Abstract

The present invention is directed to serve ligand screening apparatuses, ligand screening methods, programs and recording medium for studying the binding analysis

5   between a receptor including an induced-fit type receptor and a ligand. First, analysis and calculation of normal mode are conducted, and then fluctuation of dihedral angle of main chain in a steady state is calculated. Then by carrying out molecular dynamic calculation while imposing

10   constraint on each atom based on the fluctuation, dynamic structure of the receptor is predicted more accurately. By using the dynamic structure obtained in the molecular dynamic calculation and an interaction function, receptor/ligand binding which is also applicable to an

15   induced-fit type receptor is predicted with high accuracy.